

Electronic and lattice dynamical properties of the iron-based superconductors LiFeAs and NaFeAs

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The electronic structure and lattice vibrational frequencies of the newly discovered superconductors, LiFeAs and NaFeAs, are calculated within density functional theory. We show that in the vicinity of the Fermi energy, the density of states is dominated by contributions from Fe 3d states. We also calculate the electron-phonon coupling strength and show that it is too weak to account for the observed values of the superconducting transition temperatures. This seems to indicate that the iron-based superconductors are not of the conventional type.

I. INTRODUCTION

A new class of layered, high- T_c superconductors has been recently discovered. Kamihara et al.^{1,2} reported a superconducting transition temperature $T_c=26$ K in fluorine-doped LaOFeAs. Shortly afterwards, it was found that under pressure T_c increased to 43 K.³ Replacement of lanthanum with other rare earth metals gave a series of superconducting compounds $\text{ReO}_{1-x}\text{F}_x\text{FeAs}$, where Re = Ce, Pr, Nd, Sm, or Gd, with transition temperatures close to or exceeding 50 K.^{4,5,6,7,8,9} Oxygen deficient samples were also synthesized and found to superconduct at 55 K.^{10,11,12} Hole doping, through the partial substitution of La with Sr, or Gd with Th, was also found to yield superconducting compounds.^{13,14} Using high pressure techniques, it was possible to increase the concentration of the F-dopant¹⁵ and to synthesize superconducting compounds where La is replaced by the late rare earth elements Tb and Dy.^{16,17} The parent compound ReOFeAs is a layered compound consisting of a stack of alternating ReO and FeAs layers. Each ReO layer consists of an O-sheet surrounded by two Re sheets. Similarly, each FeAs layer consists of an Fe-sheet surrounded by two As sheets such that each Fe atom is tetrahedrally coordinated to four As atoms. Neutron diffraction measurements^{18,19,20,21} establish that the Fe magnetic moments adopt a collinear antiferromagnetic (c-AFM) order whereby ferromagnetic chains are coupled antiferromagnetically along the direction orthogonal to the chains.

Superconductivity was also discovered in a second class of compounds containing FeAs layers, namely AFe_2As_2 , where A is an alkaline earth metal. Hole doping, by partial replacement of A with alkali metals, results in superconducting compounds with T_c reaching 38 K in BaFe_2As_2 and SrFe_2As_2 .^{22,23,24,25,26} Partial substitution of Fe with Co was also shown to give a superconducting compound with $T_c=22$ K.²⁷ Similarly to the first class, in the parent compounds the Fe magnetic moments in this second class have a collinear AFM order with a spin-stripes pattern.^{28,29,30} In both classes, the Fe magnetic moments in the parent compounds exhibit magnetic order, at low temperature, which disappears upon doping, making way for the emergence of superconductivity. This

leads to the reasonable belief that strong electronic correlations are important in these systems, and that superconductivity in these compounds is somehow connected to magnetic fluctuations.^{31,32,33,34,35,36,37,38,39,40,41,42,43} Indeed, the electron-phonon coupling in LaOFeAs was estimated to be too small⁴⁴ to give rise to superconductivity within the conventional BCS formulation.⁴⁵

Recently, a third class of iron-based superconductors was discovered. LiFeAs and NaFeAs were found to superconduct below 18 K and 9 K, respectively.^{46,47,48,49} It turns out that in these two compounds, no magnetic order is detected at all temperatures. In some sense, these two compounds are important with regards to understanding the mechanism of superconductivity in iron-based superconductors. the absence of spin density wave (SDW) transition, on the one hand, and the relatively low T_c in comparison with the first two classes of iron-based superconductors, on the other hand, make these two compounds possible candidates for being conventional BCS superconductors.

Band structure calculations, using local density approximation (LDA) within density functional theory (DFT), were recently reported for LiFeAs.^{50,51} It was found that LiFeAs is semi-metallic, and that the density of states (DOS) near the Fermi level is dominated by the Fe 3d states. Thus, the electronic structure of stoichiometric LiFeAs is similar to that of the parent compounds of the first class, with a hole cylinder at the Brillouin zone (BZ) center, electron cylinders at the BZ corners, and an electronic DOS that decreases strongly with increasing energy in the vicinity of the Fermi energy.

In this work we report DFT calculations of the electronic and lattice properties of LiFeAs and NaFeAs. In particular, we calculate the electron-phonon coupling strength and show that it is too weak to account for the superconducting transition temperatures observed in these compounds. Our calculations, together with previous calculations⁴⁴ of the electron-phonon coupling strength in LaOFeAs, seem to indicate that iron-based superconductors are not of the conventional type.

II. METHOD

The electronic structure calculations are carried out using the all-electron full-potential linear augmented plane wave (FP-LAPW) method as implemented in WIEN2K code.⁵² The exchange-correlation potential was calculated using the generalized gradient approximation (GGA) as proposed by Pedrew, Burke, and Ernzerhof (PBE).⁵³ The radii of the muffin-tin spheres for the various atoms were chosen so that the neighboring spheres almost touch each other. We set the parameter $R_{MT}K_{max}=7$, where R_{MT} is the smallest muffin-tin radius and K_{max} is a cutoff wave vector. The valence wave functions inside the muffin-tin spheres are expanded in terms of spherical harmonics up to $l_{max} = 10$, and in terms of plane waves with a wave vector cutoff K_{max} in the interstitial region. The charge density is Fourier expanded up to $G_{max}=13a_0^{-1}$, where a_0 is the Bohr radius. Convergence of the self-consistent field calculations is attained with a total energy convergence tolerance of 0.01 mRy.

The calculation of the frequencies of the vibrational modes and the electron-phonon coupling parameter was performed using ultrasoft pseudopotentials and an expansion of the wave function of the valence electrons in terms of plane waves, with an energy cutoff of 30 Rydbergs.⁵⁴ In both the electronic and lattice calculations, the experimental values of the low-temperature lattice constants and atomic positions^{46,49} are used. For both compounds, the crystal is tetragonal with space group P4/nmm. In LiFeAs, the lattice constants are $a = 3.76982 \text{ \AA}$, $c = 6.30693 \text{ \AA}$, whereas in NaFeAs, $a = 3.94729 \text{ \AA}$, and $c = 6.99112 \text{ \AA}$.

III. RESULTS AND DISCUSSION

Our results for the electronic structure calculations for LiFeAs and NaFeAs are summarized in figures 1 and 2, respectively, where the electronic density of states (DOS) is displayed. For LiFeAs, our calculated DOS is similar to that reported earlier.^{50,51} In both LiFeAs and NaFeAs, the DOS plots show some generic features that are common to the parent compounds of the iron-based superconductors: A DOS that is dominated by the Fe 3d states in the vicinity of the Fermi energy, with only a small contribution from the As and alkali metal states, and that is strongly decreasing with energy near the Fermi energy. It should be noted that in a unit cell of LiFeAs, for example, there are two Li, two Fe, and two As atoms. Thus to get the total atomic DOS, the values of the atomic DOS shown in 1 should be multiplied by 2. The total DOS is the sum of the total atomic DOS and the DOS in the interstitial region.

Since the DOS at the Fermi energy, $N(E_F)$, is ~ 4 states/eV in both LiFeAs and NaFeAs, which is not very small, and because of the relatively lower T_c compared with the other iron-based superconductors, one may won-

der whether electron-phonon coupling may lie behind the mechanism for superconductivity in LiFeAs and NaFeAs. This notion may be given more credence by the observation that a sodium atom is about three times more massive than a lithium atom, so that if the attractive electron-electron interaction is mediated by the alkali-metal atomic vibrations, then this difference in the mass could explain the difference in the values of T_c between the two compounds via the well-known isotope effect.

To test this idea, we carried out a calculation of the phonon dispersion curves and the electron-phonon coupling strength in these compounds. Since the crystallographic point group in LiFeAs and NaFeAs is D_{4h} , the vibrational modes at Γ , the BZ center, are decomposed according to the following irreducible representations

$$\Gamma_{phonon} = 2A_{1g} + B_{1g} + 3E_g + 3A_{2u} + 3E_u.$$

The acoustic modes, with vanishing frequency at Γ , the BZ center, transform according to the A_{2u} and E_u irreducible representations. Excluding the acoustic modes, we are left with 15 modes with nonzero frequencies; among these, the symmetric ones are Raman-active, while the antisymmetric modes are infrared-active. The calculated frequencies of the Raman- and infrared-active modes at the Γ point of the BZ are given in Table I. The phonon dispersion curves in LiFeAs, plotted along high symmetry directions in the BZ, are shown in Fig. 3, and the corresponding curves in NaFeAs are given in Fig. 4. Our results for the phonon frequencies at the BZ center may be checked by Raman scattering and infrared absorption experiments, while the phonon dispersion curves may be checked by neutron scattering measurements.

We calculated the electron-phonon coupling parameter λ and found it to be 0.29 and 0.27 for LiFeAs and NaFeAs, respectively. For conventional superconductors, where the attractive electron-electron interaction is mediated by phonons, the transition temperature is given by the Allen and Dynes⁵⁵ modified McMillan's formula⁵⁶

$$T_c = \frac{\omega_{log}}{1.2} \exp\left[\frac{-1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right]$$

where ω_{log} is the logarithmic average phonon frequency, expressed in degrees Kelvin, and μ^* is the Coulomb pseudopotential parameter, usually taken to be ~ 0.13 . Since ω_{log} in LiFeAs and NaFeAs is of the order of 100 K, the resulting value of T_c is much less than 1 K. We conclude that the electron-phonon coupling is too weak to account for superconductivity in this class of iron-based superconductors.

There are some puzzling questions that beset this third class of iron-based superconductors. In the parent compounds of the first two classes of iron-based superconductors, magnetic order is established at low temperatures, where the Fe magnetic moments adopt a collinear antiferromagnetic (c-AFM) order; this is unequivocally confirmed by both neutron

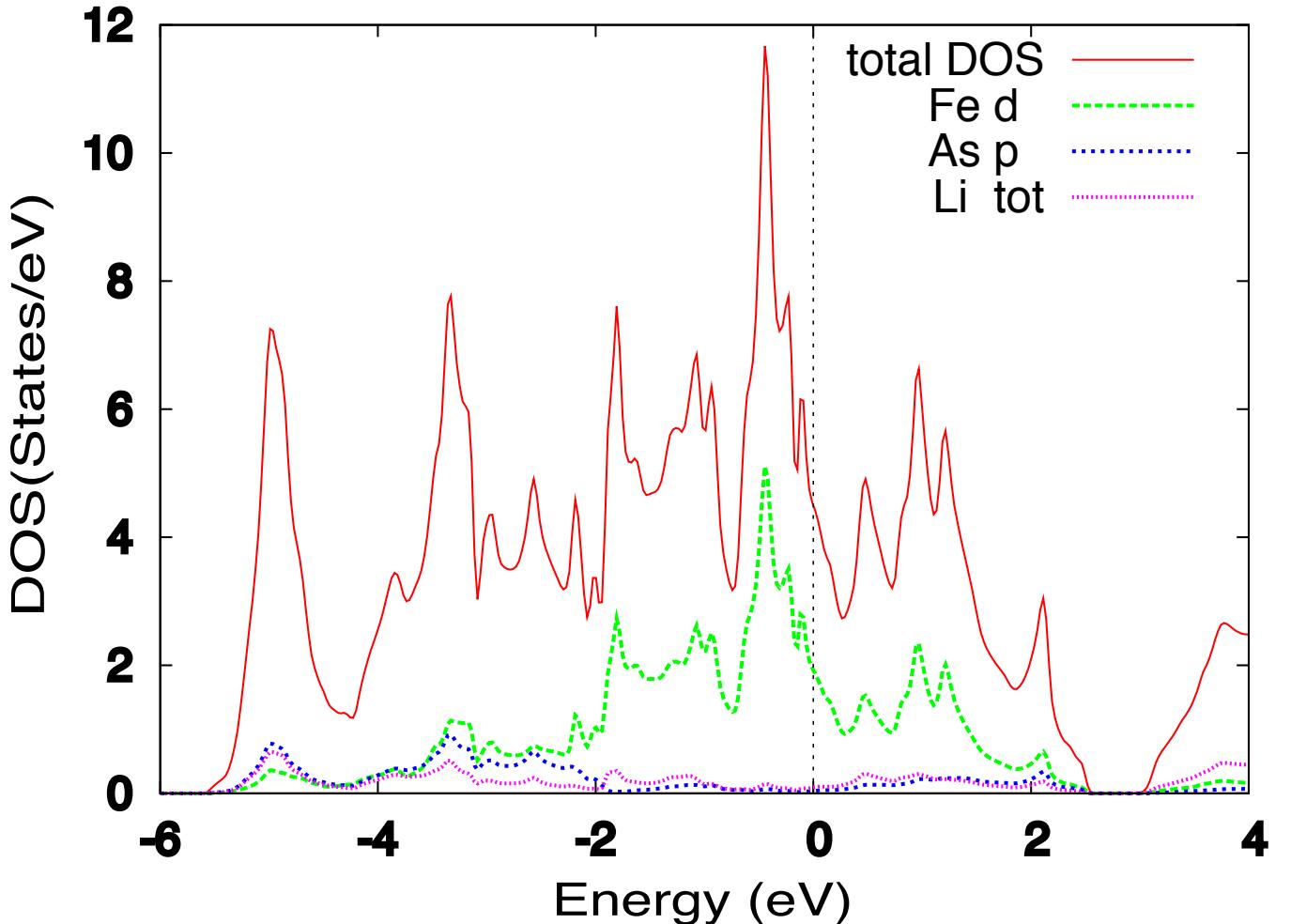


FIG. 1: (Color online) Density of states (DOS) in LiFeAs. Both the total and atomic DOS are shown. The Fermi energy is the zero energy. Near the Fermi energy, the DOS is dominated by the Fe 3d states.

TABLE I: The calculated frequencies, in cm^{-1} , of the Raman- and infrared (IR)-active modes in LiFeAs and NaFeAs. The modes are classified by the irreducible representations (irreps) according to which they transform.

		$\omega(\text{irrep})/\text{cm}^{-1}$					
		121(E _g)	188(A _{1g})	225(B _{1g})	240(E _g)	294(E _g)	356(A _{1g})
LiFeAs	Raman	121(E _g)	188(A _{1g})	225(B _{1g})	240(E _g)	294(E _g)	356(A _{1g})
	IR	228(E _u)	276(E _u)	277(A _{2u})	338(A _{2u})		
NaFeAs	Raman	110(E _g)	176(A _{1g})	187(E _g)	199(A _{1g})	218(B _{1g})	241(E _g)
	IR	170(E _u)	183(A _{2u})	233(E _u)	253(A _{2u})		

diffraction measurements^{18,19,20,21} and DFT calculations.^{32,33,34,35,36,37,38,39,40} In the first class, it is only upon electron doping through the replacement of a small percentage of oxygen atoms with fluorine atoms, or the removal of a small percentage of oxygen atoms, that the magnetic order is suppressed and superconductivity emerges. In the second class of iron-based superconductors, magnetic order is suppressed by hole doping through the replacement of some alkaline earth atoms with alkali

atoms. To better understand the situation in the third class of iron-based superconductors, we carried out spin-polarized DFT calculations on stoichiometric LiFeAs and NaFeAs, in addition to the calculations reported above for the nonmagnetic phases of these compounds. We considered, within GGA and GGA+U, various spin arrangements on the Fe sites. Similarly to the case of the first two classes, we find that the c-AFM phase, with a spin-stripes pattern, is indeed the lowest energy phase. Within GGA,

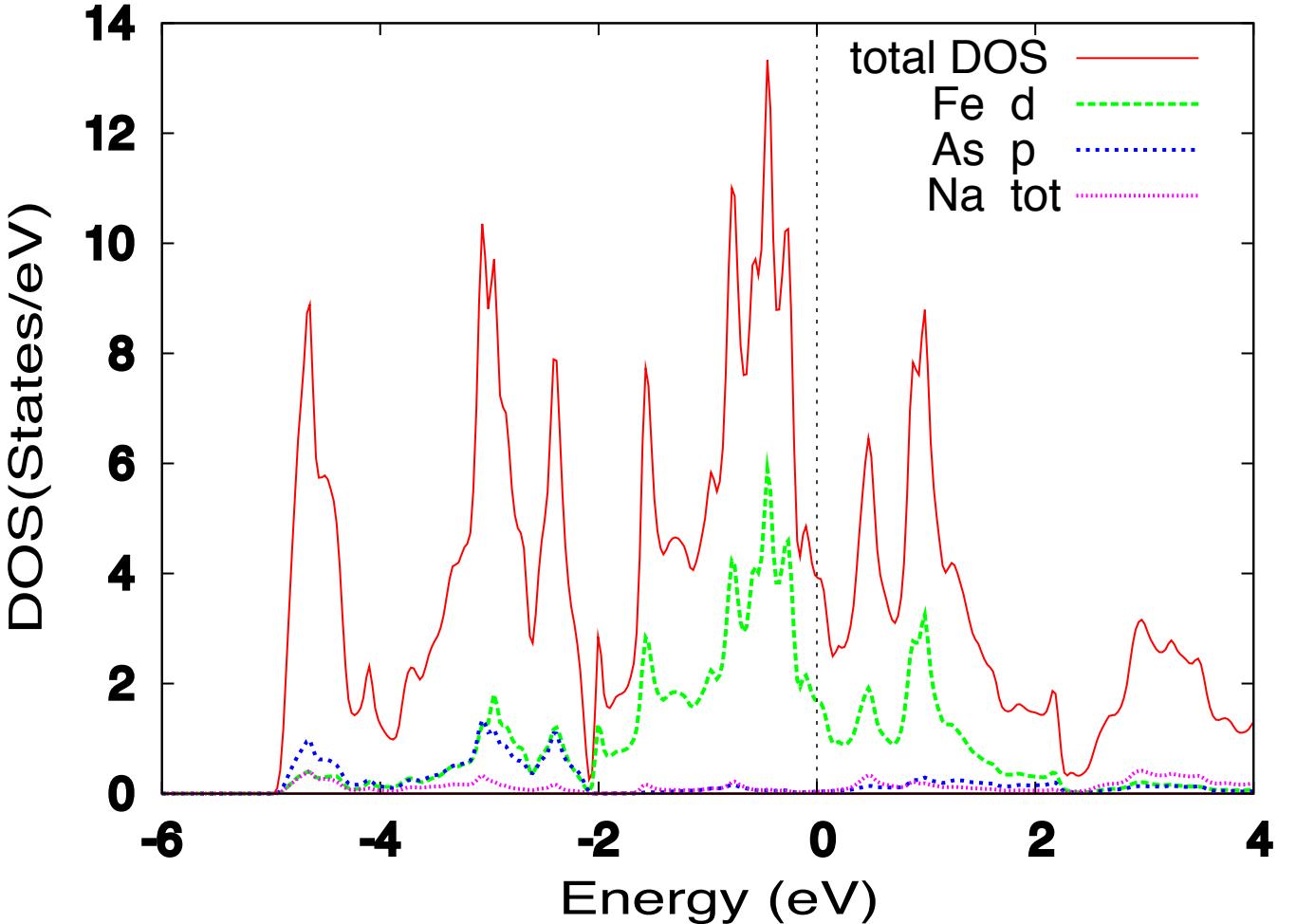


FIG. 2: (Color online) Density of states (DOS) in NaFeAs. Both the total and atomic DOS are shown. The Fermi energy is the zero energy. Near the Fermi energy, the DOS is dominated by the Fe 3d states.

the energy of the c-AFM phase in LiFeAs is lower than the AFM phase by 0.081 eV per Fe atom (eV/Fe), lower than the ferromagnetic (FM) phase by 0.085 eV/Fe, and lower than the nonmagnetic phase by 0.123 eV/Fe. For NaFeAs, the energy of the c-AFM phase is lower than the AFM phase by 0.048 eV/Fe, lower than the FM phase by 0.205 eV/Fe, and lower than the nonmagnetic phase by 0.182 eV/Fe. The differences are even greater within GGA+U, where onsite Coulomb repulsion is taken into account. Thus, according to our DFT calculations, stoichiometric LiFeAs and NaFeAs should be similar to the parent compounds of the first two classes, and they should not superconduct; instead, at low temperature, the stoichiometric compounds should display magnetic order. Deviations from stoichiometry, on the other hand, may suppress the magnetic order, making way for superconductivity, just like doping does in the first two classes of iron-based compounds. In the case of LiFeAs, it is indeed the case that the synthesized superconducting compounds were not stoichiometric, the chemical formula being $\text{Li}_{1-x}\text{FeAs}$.⁴⁸ The situation is less clear in the case

of NaFeAs,⁴⁹ but we believe, on the basis of our spin-polarized calculations, and the absence of any detectable magnetic order at low temperatures, that the synthesized NaFeAs samples must also be nonstoichiometric, and that further studies on sample characterization are necessary in this regards.

IV. CONCLUSIONS

In conclusion, we have presented the results of electronic structure calculations on LiFeAs and NaFeAs, members of a new class of superconducting compounds. In similarity to other iron-based superconductors, the density of states in the vicinity of the Fermi energy is found to be dominated by contributions from the Fe 3d states. We have also calculated the Raman and infrared phonon frequencies at the Brillouin zone center, as well the phonon dispersion curves along high symmetry directions in the Brillouin zone. We have evaluated the electron-phonon coupling parameter in LiFeAs

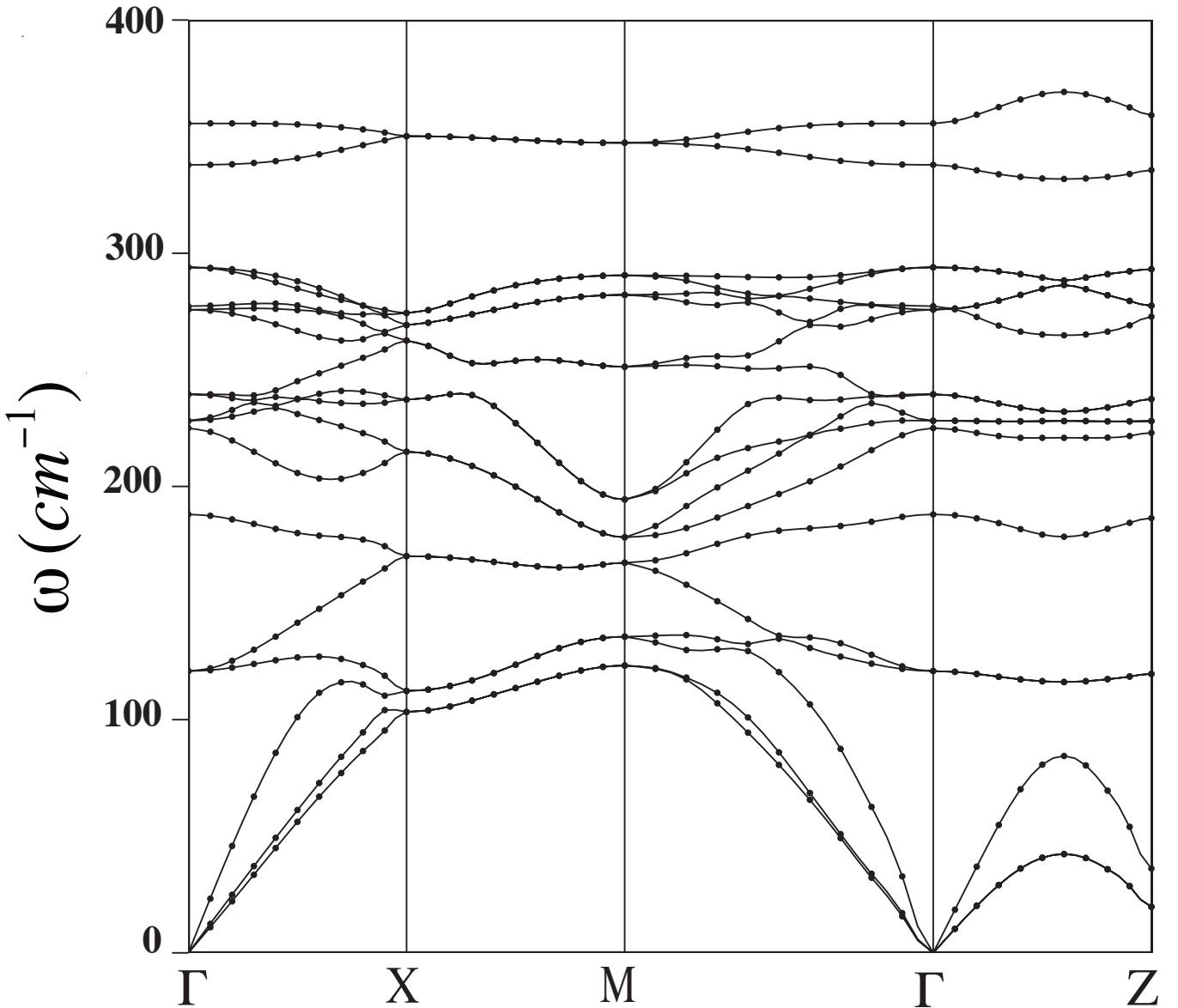


FIG. 3: Phonon dispersion curves in LiFeAs, plotted along high symmetry directions of the Brillouin zone.

and NaFeAs, and found its value to be too small to account for the observed superconducting transition temperatures in these compounds. Our results, taken together with previous estimates of the electron-phonon

coupling strength in LaOFeAs, seem to suggest clearly that iron-based superconductors are not of the conventional type, where the attractive electron-electron interaction is mediated by phonons.

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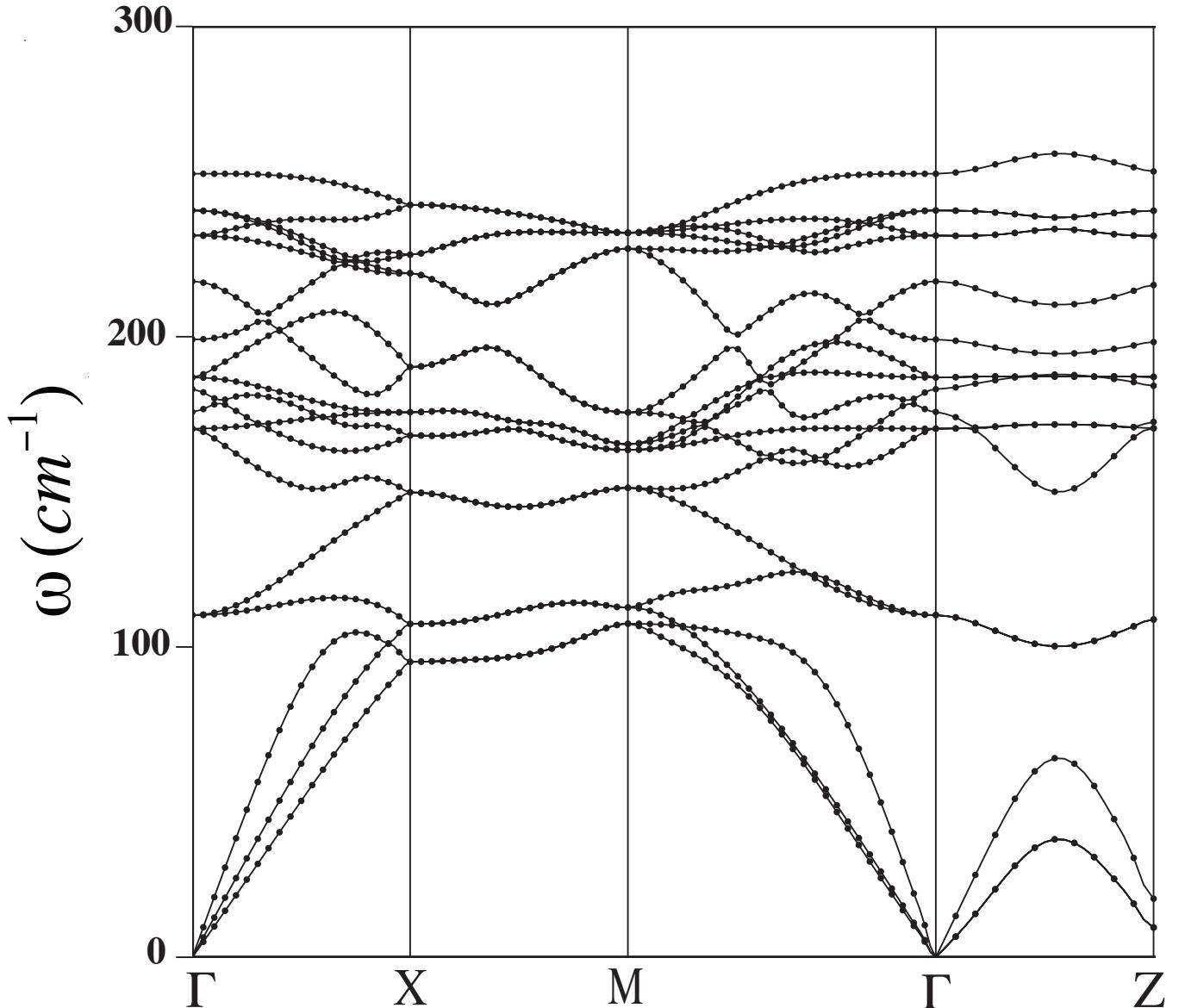


FIG. 4: Phonon dispersion curves in NaFeAs, plotted along high symmetry directions of the Brillouin zone.

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